Local lattice symmetry of spin-glass and antiferromagnetic URh_2Ge_2

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Abstract

Polarized x-ray absorption fine-structure (XAFS) data are reported for Rh and Ge K edges on antiferromagnetic and spin-glass samples of URh_2Ge_2. Proposed crystal structures have two possible kinds of layers for the Rh and Ge atoms. The XAFS data indicate that each species occupies both kinds of layers, indicating that the dominant phase has a crystal structure like that of $CaBe_2Ge_2$.

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The physical properties of URh_2Ge_2 are interesting both from the point of view of a uranium-containing, heavy-fermion spin glass, and because this material has many properties in common with disordered non-Fermi liquids (NFL) [1], potentially indicating that the root of this behavior is similar to that of some NFL's. URh_2Ge_2 forms most easily into a spin glass (T_F=9 K), but simple annealing can transform it into an antiferromagnet (T_N=13.4 K) [1], providing evidence that lattice disorder generates the magnetic disorder necessary for the spin-glass phase. In order for real comparisons to other spin glasses and NFL's to be made, the microscopic details of this system's unexpected lattice disorder need to be understood. In particular, even the average crystal symmetry is only tentatively identified as $P4/nmm$ [2] ($CaBe_2Ge_2$-like), with $I4/mmm$ ($ThCr_2Si_2$-like) among the other candidate structures. Below, we refer to these as the AS (assymetrically-stacked) and the SS (symmetrically-stacked) models.

The x-ray absorption fine-structure (XAFS) technique can help clarify the situation. The Fourier transform (FT) of the normalized fine structure (χ) above an absorption edge is closely related to the radial bond length distribution around the absorbing atom. Moreover, since the final state of the photoelectron for a K edge has p symmetry, the XAFS have a directional dependence with respect to the incident photon polar-

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ization, $\hat{\boldsymbol{\epsilon}}$. Specifically, the XAFS amplitude is proportional to $(\hat{\boldsymbol{\epsilon}} \cdot \boldsymbol{r}_i)^2$, where $\boldsymbol{r}_i$ points along the direction to a neighboring atom. This feature has certain advantages when considering a non-cubic crystal, such as the one in Fig. 1a. For instance, by rotating the crystal with respect to $\hat{\boldsymbol{\epsilon}}$, one can enhance or remove signal corresponding to the near-neighbor pairs within the r-type layers. In this way, we can determine whether the Rh atoms sit only in r-type layers as in the SS model, or whether they also occupy s-type layers, as in the AS model.

Data were collected in the fluorescence mode on single crystals of spin-glass and antiferromagnetic samples at 30 K from the Rh and Ge K edges. The samples were rotated within 10° of $\hat{\boldsymbol{\epsilon}}//\boldsymbol{c}$ and again within 10° of $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$. Figure 1b shows FEFF8 [3] simulations of the Rh K-edge data with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$ for the two proposed models (lattice vibrations only roughly included, lattice constants from Ref. [2]). The main peak at ~2.2 Å is due to the Rh-Ge near neighbors between the s- and r-type layers, corresponding to a pair distance of about 2.5 Å. The next peak at ~2.6 Å in the transform is due to the Rh-Rh pairs within r-type layers with a bond length of about 2.9 Å. This latter peak is not present with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{c}$ for either the simulated or the measured data (not shown). In the SS simulation, all the Rh is in r-type layers, and the Rh-Rh (2.9 Å) scattering is maximized. In the AS simulation, this amplitude is half that of the SS simulation, since half the Rh atoms are in s-type layers. The measured data [4] shown in Fig. 1c clearly has amplitude in this region of the transform that is more consistent with the AS simulation, and fits assuming the AS model are excellent. Moreover, the data from both orientations and from the Ge K edge support the AS model over the SS model. A third possibility that allows for both Rh and Ge atoms in a single layer is also ruled out as the dominant phase, since the first large peak from the Rh (Ge) edge data is found to be predominantly Ge (Rh). This random-occupancy phase may partially account for any impurity phases, however. The data and results on the spin glass sample are very similar.

In conclusion, the XAFS data on both antiferromagnetic and spin-glass sampes are consistent with

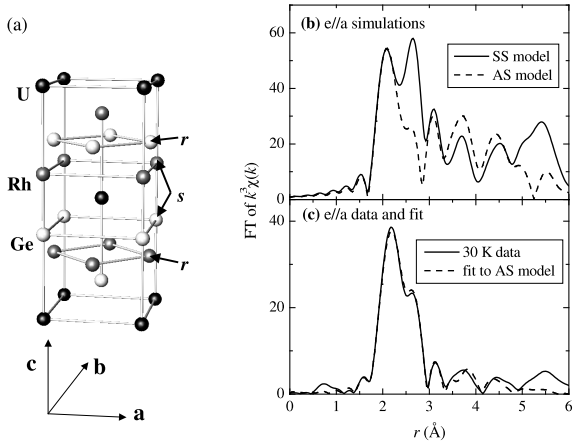

Fig. 1. (a) The proposed AS model for URh_2Ge_2. The SS-model structure is similar, with Ge occupying only s-type layers and Rh occupying only r-type layers. (b) Simulations of the Rh K-edge data with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$ assuming the two proposed lattice models. (c) Data on the antiferromagnetic sample with a fit to the AS model.

the dominant crystal phase of URh_2Ge_2 having Rh and Ge alternate between s- and r-type layers. Although XAFS is not sensitive to long-range structure, this stacking is like that of $CaBe_2Ge_2$. This lattice is unusual for the f-electron intermetallic 122's, which are usually like that of $ThCr_2Si_2$. Disorder relative to this phase as well as differences between the antiferromagnetic and spin-glass samples will be the topic of a future paper.

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